

Casimir Effect for Massless Fermions in One Dimension: A Force Operator Approach

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We calculate the Casimir interaction between two short range scatterers embedded in a background of one dimensional massless Dirac fermions using a force operator approach. We obtain the force between two finite width square barriers, and take the limit of zero width and infinite potential strength to study the Casimir force mediated by the fermions. For the case of identical scatterers we recover the conventional attractive one dimensional Casimir force. For the general problem with inequivalent scatterers we find that the magnitude and sign of this force depend on the relative spinor polarizations of the two scattering potentials which can be tuned to give an attractive, a repulsive, or a compensated null Casimir interaction.

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Boundaries modify the spectrum of zero point fluctuations of a quantum field, resulting in fluctuation-induced forces and pressures on the boundaries that are known generally as Casimir effects [1]. When sharp boundaries conditions are used to model the Casimir effect, they yield perfect reflection of the incident propagating quantum field at all energies [1]. However, in many physical applications this hard-wall limit is not appropriate; of special interest in the present work are interactions between localized scatterers in one dimension that have energy-dependent scattering properties controlled by the strength, range and shape of the potential. Along this line, previous work has recognized that the finite reflectance of partially transmitting mirrors provides a natural high energy regularization scheme for computing the effect of sharp reflecting boundaries on the zero point energy of the electromagnetic field [2, 3]. In more recent work, Sundberg and Jaffe approached the problem of computing the effect of confining boundary conditions on a degenerate gas of fermions in one dimension as the limiting behavior for rectangular barriers of finite width and height. Interestingly, they encounter a divergence of the Casimir energy in the zero width limit (a sharp boundary) even for finite potential strength [4].

In this Rapid Communication we address the problem of Casimir interactions between scatterers mediated by a one-dimensional Fermi gas. The fermions in our calculation are massless Dirac fermions appropriate to describe, for example, the (single-valley) electronic spectrum of a metallic carbon nanotube. We employ the Hellmann-Feynman theorem to calculate the force, rather than energy, of interaction between two scatterers as a function of their separation d . This approach renders our calculation free from ultraviolet divergences even for the limiting case of sharp scatterers. We demonstrate that for the case of identical scatterers, this formalism recovers the well known attractive $1/d^2$ Casimir force in one dimension. Furthermore, we find that for Dirac fermions the internal structure of the matrix-valued scattering po-

tential admits a long range Casimir interaction which can also be repulsive or even compensated. This provides a physical situation where the Casimir interaction is continuously tunable from attractive to repulsive by variation of an internal control parameter, realizing the known bounds for the one dimensional Casimir interaction as two limiting cases. The results may be relevant for indirect interactions between defects and adsorbed species on carbon nanotubes.

The fermions in our model are massless one-dimensional Dirac fermions described by the Hamiltonian

$$(-i\sigma_x\partial_x + \hat{V}(x) - E)\Psi_k(x) = 0, \quad (1)$$

where we set $\hbar = c = 1$. In graphene and carbon nanotubes the spinor polarizations describe the internal degrees of freedom generated by the two-sublattice structure in its primitive cell. When $\hat{V}(x) = 0$, the eigenstates of \mathcal{H}_0 are plane waves multiplying two-dimensional spinors, $\Psi_k(x) = \Phi_k e^{ikx}/\sqrt{2\pi}$. When the chemical potential is fixed at $\mu = 0$, the filled Dirac sea has $E = -|k|$ with $\Phi_{\pm k}^T = (1, \mp 1)/\sqrt{2}$.

The general form of the potential entering (1) is $\hat{V}(x) = V_0(x)\hat{I} + \vec{V}(x) \cdot \vec{\sigma}$. The σ_x part of the potential can be eliminated by a gauge transformation [4], and a scalar potential proportional to the identity matrix produces no backscattering in the massless Dirac equation. Therefore, we consider potentials for which \vec{V} lies in the yz -plane. In this paper, we consider the effects of the orientation of the potential determined by angle ϕ . Thus, a square barrier potential located between points x_1 and x_2 is written as

$$\hat{V}(x, \phi) = \hat{V}(\phi)\theta(x - x_1)\theta(x_2 - x), \quad (2)$$

where $\hat{V}(\phi) = V e^{i\sigma_x\phi/2}\sigma_z e^{-i\sigma_x\phi/2}$, and $\theta(x)$ is a step function.

To study the force on a square well scatterer we use the Hellmann-Feynman theorem, $\langle \partial \mathcal{H}(\lambda) / \partial \lambda \rangle = \partial E / \partial \lambda$ [5]. Taking the control parameter $\lambda = (x_1 + x_2)/2 = \bar{x}$,

the ground state average gives the force acting on a rigid barrier. For a barrier with sharp walls the expectation value becomes

$$\langle \Psi(x) | \frac{\partial \hat{\mathcal{H}}}{\partial \bar{x}} | \Psi(x) \rangle = \langle \Psi(\bar{x} + a/2) | \hat{V} | \Psi(\bar{x} + a/2) \rangle - \langle \Psi(\bar{x} - a/2) | \hat{V} | \Psi(\bar{x} - a/2) \rangle, \quad (3)$$

where \hat{V} is the square barrier potential, \bar{x} is its center and a is its width. The total force is the expectation value of this force operator, $\hat{F} = -\partial \hat{\mathcal{H}} / \partial \bar{x}$, summed over all the occupied states; Eq. (3) then gives the difference between the pressures exerted on the right and the left sides of the barrier. For potentials of general shape a similar expression can be developed in terms of an integral over the scattering region.

First, we apply Eq. (3) to calculate the force on an isolated barrier. The eigenstates are represented as linear combinations of right and left moving solutions of \mathcal{H}_0 : $\Psi(x) = \frac{1}{\sqrt{2\pi}}(\alpha_k \Phi_k e^{ikx} + \beta_k \Phi_{-k} e^{-ikx})$, where α_k and β_k represent the amplitudes of the counterpropagating waves in each region. The yz polarized potential defined in Eq. (2) gives $\hat{V}(\phi) \Phi_{\pm k} = V e^{\pm i\phi} \Phi_{\mp k}$, so the general expression for the expectation values in Eq. (3) at some position x is

$$\langle \Psi(x) | \hat{V}(\phi) | \Psi(x) \rangle = \frac{V}{\pi} \mathcal{R}e[\alpha_k \beta_k^* e^{i(2kx+\phi)}]. \quad (4)$$

We use a transfer matrix to obtain the coefficients α_k and β_k entering Eq. (4). The transfer matrix is defined so that $\Psi(x_2) = T \Psi(x_1)$, where x_1 and x_2 are the left and right boundaries of a barrier, respectively; T is calculated by integrating Eq. 1,

$$T = P_x \exp \left(i \int_{x_1}^{x_2} dx \sigma_x [E - \hat{V}(x)] \right), \quad (5)$$

where P_x is a spatial ordering operator. For the square potential of width a defined in Eq. (2), the transfer matrix for negative energy states is

$$T = \cos(qa) - \frac{i\sigma_x k - \vec{\sigma} \cdot (\hat{x} \times \vec{V})}{q} \sin(qa), \quad (6)$$

where $\vec{V} = V(0, \sin \phi, \cos \phi)$ defines a potential in the yz -plane, $q = \sqrt{k^2 - V^2}$, and $k > 0$.

From the transfer matrix we calculate the scattering matrix S , which gives the transmitted (t) and reflected (r) amplitudes for wave incident on the barrier from the right and from the left. The unitary S-matrix for a single square barrier is

$$S_1 = \begin{pmatrix} t e^{-ika} & r e^{-i(2kx_2+\phi)} \\ r e^{i(2kx_1+\phi)} & t e^{-ika} \end{pmatrix}. \quad (7)$$

The transmission and reflection coefficients can then be parameterized $t = \tau e^{i\eta}$ and $r = i\sqrt{1 - \tau^2} e^{i\eta}$, where

$$\tau = \frac{\lambda}{(V^2 \cosh^2 \lambda a - k^2)^{1/2}}, \eta = \tan^{-1} \left(\frac{k \tanh \lambda a}{\lambda} \right), \quad (8)$$

with $\lambda = -iq = \sqrt{V^2 - k^2}$. To obtain the hard-wall limit, we fix $\Gamma = Va$, and take $\Gamma \rightarrow \infty$. In this limit, $|r|^2 \rightarrow 1$ and $|\eta|^2 \rightarrow 0$ at all energies.

For a single barrier, the contributions to the force from the particles incoming from the right and the left cancel, resulting in no net force. A nonzero force arises from the multiple reflection of electron waves between two barriers. An illustration of a scattering process for two square potentials with different spinor polarizations ϕ_1 and ϕ_2 separated by distance d is shown in Fig. 1. The contributions from waves incoming from the right are also included in the calculation.

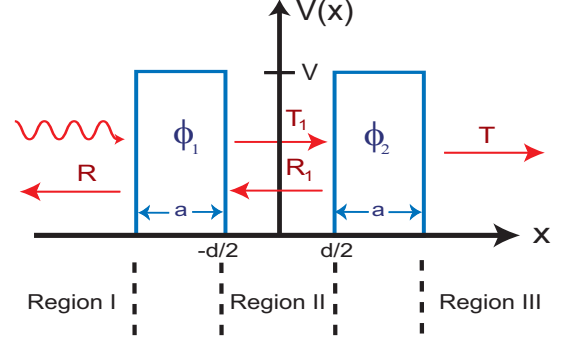


FIG. 1: Scattering of massless Dirac fermions (incoming from the left) between two square barriers of height V , width a , and separation d . The two potentials defined in Eq. (2) have a spinor polarization determined by angle ϕ . The reflection and transmission coefficients are labeled in each scattering region.

The S-matrix for the two-barrier system [6] in Fig. 1 is

$$S_2 = \begin{pmatrix} T & R e^{i\phi_1} \\ R e^{-i\phi_2} & T \end{pmatrix}. \quad (9)$$

The total reflection and transmission coefficients shown in regions I and III of Fig. 1 are given by

$$T = \frac{t^2}{1 - r^2 e^{i\nu}}, \quad R = r e^{-ik(2a+d)} \left(1 + \frac{t^2 e^{i(2ka+\nu)}}{1 - r^2 e^{i\nu}} \right), \quad (10)$$

where $\nu = 2kd + \delta\phi$ and $\delta\phi \equiv \phi_2 - \phi_1$. T_1 and R_1 in region II of Fig. 1 are given by

$$T_1 = \frac{t}{1 - r^2 e^{i\nu}}, \quad R_1 = \frac{r t e^{i(kd+\phi_2)}}{1 - r^2 e^{i\nu}}. \quad (11)$$

The coefficients for the waves incoming from the left (R_1 and T_1), and the ones incoming from the right (R'_1 and T'_1) are related by $R'_1 = R_1 e^{-i(\phi_1+\phi_2)}$ and $T'_1 = T_1$.

To calculate the force in the two-barrier problem we fix the position of the left barrier in Fig. 1 and differentiate the Hamiltonian with respect to d . To obtain the total force, we sum over the occupied states of the filled Dirac sea at fixed chemical potential. We find that the force

between two square barriers of finite height and width is

$$F = -2V \int_0^\infty \frac{dk}{2\pi} \mathcal{R}e[R e^{ik(d+2a)} - R_1 T_1^* e^{-i(kd+\phi_2)}(1 + e^{i\nu})]. \quad (12)$$

The first term in the integrand arises from the exterior modes pushing the two barriers together. The second term accounts for the confined modes in between the barriers pushing them apart. Since incoming waves are fully transmitted at high energies for barriers of finite height and width, the integral in Eq. (12) converges even in the case of sharp barriers ($a \rightarrow 0$), with $\Gamma = Va$ fixed. Thus, the reflection coefficient provides a natural cutoff for the computation of the force (though not the energy [4]) even in the limit of infinitely high barriers.

The Casimir force for hard-wall boundary conditions requires the limits of infinite barrier strength $\Gamma \rightarrow \infty$ and zero width $a \rightarrow 0$. This limit enforces a vanishing current at the boundaries, the so-called bag boundary conditions. Since the force in Eq. (12) is multiplied by V , we keep terms to $\mathcal{O}(k/V)$ in the integrand. The first term in Eq. (12) becomes proportional to k , thus implying a continuous spectrum of modes scattering off the barriers from the outside. The second term exhibits resonances that arise from the quantized modes between the boundaries. These resonances, similar to ones seen in Fabry-Perot cavities, are represented by Dirac delta functions [3] to constrain the k integration

$$\lim_{\tau \rightarrow 0} \frac{\tau^2}{|1 + (1 - \tau^2)e^{i(\nu+2\eta)}|^2} = \frac{\pi}{2d} \sum_{n=0}^{\infty} \delta(k - k_n), \quad (13)$$

where $k_n = \pi[n + (1 - \delta\phi/\pi)/2]/d$, and $\eta \rightarrow 0$ in the limit of infinite potential strength. Here $\delta\phi$ is the difference in the spinor polarizations of the two scattering potentials, and $\delta\phi = 2\pi n$ denotes the situation for identical scatterers. An incoming wave vector satisfying the resonance condition in Eq. (13) gets fully transmitted through the two-barrier system. The modes in between the barriers, on the other hand, are fully reflected yielding the appropriate quantization condition. Combining these results we obtain

$$F = 2 \int_0^\infty \frac{dk}{2\pi} k \left[1 - \frac{\pi}{d} \sum_{n=0}^{\infty} \delta(k - k_n) \right] + \mathcal{O}\left(\frac{1}{V}\right). \quad (14)$$

The Casimir force in Eq. (14) can be calculated by applying the generalized Abel-Plana formula,

$$\int_0^\infty t dt - \sum_{n=0}^{\infty} (n + \beta) = - \int_0^\infty t dt \left(\frac{\sinh(2\pi t)}{\cos(2\pi\beta) - \cosh(2\pi t)} + 1 \right), \quad (15)$$

which is valid for $0 \leq \beta < 1$. Due to the rapid convergence of the integral in Eq. (15), the result does not

require an introduction of an explicit ultraviolet cutoff function [7]. More generally, since the reflection coefficient vanishes at high energy it will regularize the calculation of the force. Using Eq. (15) we obtain the force for two barriers satisfying bag boundary conditions,

$$F = -\frac{\pi}{24d^2} \left[1 - 3 \left(\frac{\delta\phi}{\pi} \right)^2 \right] \quad (16)$$

for $-\pi \leq \delta\phi < \pi$ beyond which it is periodic. We also explore the force between two scatterers of finite height and width. In the small barrier strength limit the force becomes

$$F = -\frac{\Gamma^2 \cos(\delta\phi)}{2\pi d^2} \left[1 + \mathcal{O}\left(\frac{a}{d}\right) \right]. \quad (17)$$

The force in the limits of $\Gamma \rightarrow \infty$ and $\Gamma \ll 1$ for $a \rightarrow 0$ is plotted for three periods in $\delta\phi$ in Fig. 2.

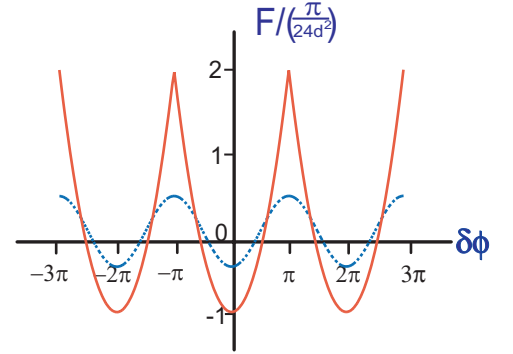


FIG. 2: Force between two barriers as a function of their relative spinor polarization $\delta\phi$. The solid and dashed lines represent the forces in Eq. (16) and Eq. (17), respectively. The magnitude of the force in the $\Gamma \ll 1$ limit, the dashed curve, is rescaled to $\Gamma = 1/2$ so the two curves can be compared.

The scaling of the force with distance as $1/d^2$ and the ratio of $1/2$ between the repulsive and attractive forces are universal results for massless one-dimensional fluctuating fields in the limit $d \gg a$. When the range of the potentials becomes comparable to their separation, the first order correction due to the shape of the scatterer scales with $\delta F/F \sim a/d$ as seen in Eq. (17), analogous to a multipole expansion of an electrostatic interaction.

The relative orientation can be expressed as $\delta\phi = \cos^{-1}(\vec{V}_1 \cdot \vec{V}_2 / (|\vec{V}_1| \cdot |\vec{V}_2|))$. When the two potentials are aligned at $\delta\phi = 2\pi n$ we have $F = -\pi/24d^2$. This yields the attractive fermionic Casimir force as found in Ref. [4]. When $\delta\phi = (2n + 1)\pi$ the relative polarization of the defect potentials is antiparallel and $F = \pi/12d^2$, i.e. a repulsive Casimir force is obtained. An analog of our result for a one-dimensional bosonic field is obtained by imposing mixed Dirichlet and Neumann boundary conditions where attractive and repulsive Casimir forces are found for like and unlike boundary conditions, respectively [9]. A Casimir force that oscillates as a function of

defect separation d is known to arise from large momentum backscattering (Friedel oscillations) of the Fermi gas [8]. However, the interaction we calculate here is monotonic as a function of distance. In our calculation, the magnitude and sign of the force varies as a function of the relative polarization of two scatters at a fixed distance. As shown in Fig. 2 this behavior occurs for both finite barriers and hard-wall boundaries.

The cusps seen in Fig. 2 at the odd multiples of n result from a sum over the discrete number of energy levels $E_n(\delta\phi)$. The energy bands found in Eq. (13) cross zero energy at $\delta\phi = (2n+1)\pi$ as shown in Fig. 3. At fixed chemical potential, with negative energy states of the Dirac sea occupied, the number of states changes by one in each 2π periodic region indicated by dotted vertical lines in Fig. 3. Consequently, the force exhibits a discontinuity in slope in Fig. 2 exactly at the values of ϕ at which there is a jump in the number of occupied energy levels. When the barrier strength is finite, the cusps in the force disappear. The resonance condition resulting in quantized states between the barriers is only valid for hard-wall boundaries. Note, the energy states between finite barriers exhibit a continuous spectrum.

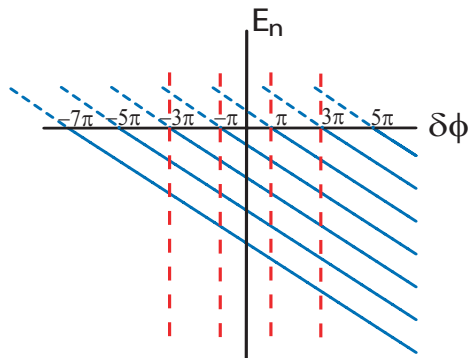


FIG. 3: Quantized energy bands for massless Dirac fermions due to hard-wall boundary conditions as a function of the relative polarization of the two potentials $\delta\phi$. Solid lines denote the energy levels of the filled Dirac sea. Vertical dashed lines define 2π periodic states where the number of occupied states changes by one.

The interaction Eq. (16) is likely to be important for defect interactions on carbon nanotubes, and possibly for other one-dimensional systems as well. Reinserting dimensional factors this force corresponds to an interaction energy $E_c = -\pi\hbar v_F/24d$ for two identical scatterers. With $\hbar v_F \sim 5.4\text{eV} \cdot \text{\AA}$ this gives an energy of 1.4meV at a range $d = 50\text{nm}$. Note that its spatial form follows the same scaling law as the Coulomb interaction between uncompensated charges, but it is reduced by a factor $\pi\hbar v_F/24e^2 \sim .05$. Thus, for charge neutral dipoles $p = es$ whose electrostatic interactions scale as $E_d \sim -p^2/d^3 = -(e^2/d) \times (s/d)^2$, they are dominated by the Casimir interaction in the far field $d \gtrsim 5s$.

Similarly, this one-dimensional Casimir interaction completely dominates the familiar van der Waals interactions between charge neutral species that are mediated by the fluctuations of the exterior three dimensional electromagnetic fields.

In order to fully understand the Casimir effect between defects on carbon nanotubes, one needs to consider the symmetry and range of the potentials produced by localized defects. The spinor polarization discussed in this paper is determined by the form of the impurity potential: σ_z and σ_y potentials define a sublattice-asymmetric and bond-centered defects, respectively. In addition, the electronic spectrum contains two distinct Fermi points at inequivalent corners of the two dimensional Brillouin zone. Short-range potentials couple the two Fermi points resulting in intervalley scattering [10]. Therefore, both the structure of the defects and the effect of intervalley scattering determine the sign and magnitude of the Casimir interaction. In the context of our model, a sharp potential is one with a range on the order of the tube radius R for which the effects of intervalley scattering are suppressed by a factor of a_c/R , where a_c is the width of the graphene primitive cell. Atomically sharp scatterers, on the other hand, will usually require a treatment of the effects of intervalley as well as intravalley scattering.

To summarize, we introduced a force operator approach for calculating the Casimir effect and obtained the fluctuation-induced force between two finite square barriers mediated by massless Dirac fermions in one dimension. In taking the limit of sharp barriers of infinite strength we obtained a Casimir force that scales as $1/d^2$, and is tunable from attractive to repulsive form as a function of the relative spinor polarizations of the two scattering potentials.

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